HIGHLY AUTOMATED MACROMOLECULAR CRYSTALLOGRAPHY BEAMLINE (AMX)

BROOKHAVEN NATIONAL LABORATORY

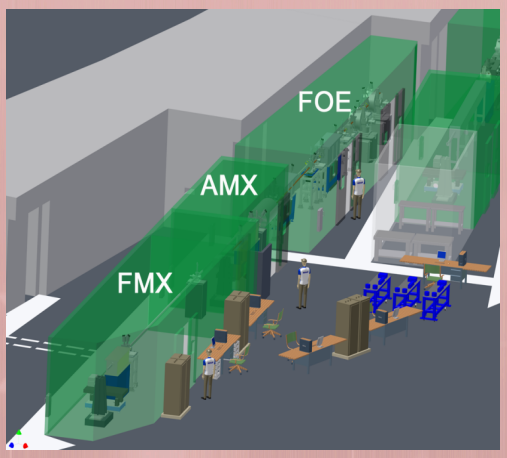
Group Leader: Dieter Schneider Proposal Team: M. Allaire[1], L. Berman[1], M. Chance[2], W. Hendrickson[3], A. Héroux[1], J. Jakoncic[1], A. Orville[1], H. Robinson[1], **D. Schneider[1]**, W. Shi[2], A. Soares[1], V. Stojanoff[1], R. Sweet[1]
[1]Brookhaven National Laboratory, [2]Case Western Reserve University, [3]Columbia University

NATIONAL SYNCHROTRON LIGHT SOURCE II • ABBIX project • funded by NIH

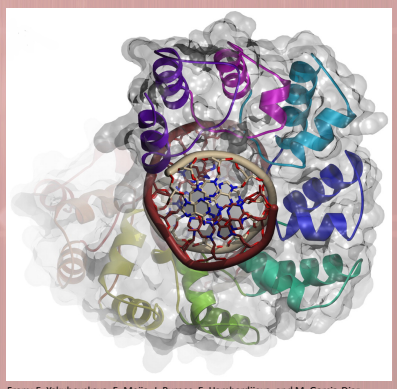
MISSION

- AMX at NSLS-II will provide structural biologists with ready access to an advanced macromolecular crystallography (MX) beamline for the elucidation of structure and function of macromolecular complexes.
- Its high flux, tunable energy, and natively small focal spot will make it a crystallographer's preferred beamline.
- Its high degree of automation will provide a high throughput capability and invite remote participation.
- AMX, together with FMX and LIX, is funded by the NIH through the ABBIX* project for the construction of biomedical beamlines. It is part of an initial suite of three specialized MX beamlines and complements the micro-focusing capabilities of FMX and the high energy-resolution capability of NYX.

*ABBIX: Advanced Beamlines for Biological Investigations with X-rays

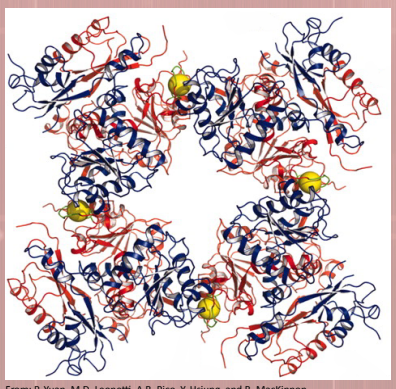


APPLICATIONS AND CAPABILITIES



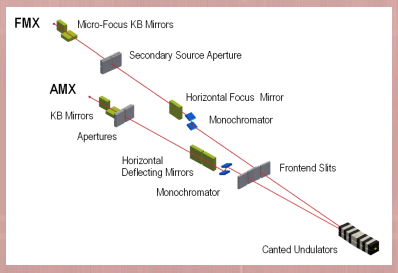
From: E. Yakubovskaya, E. Mejia, J. Byrnes, E. Hambardjieva, and M. Garcia-Diaz, Helix Unwinding and Base Flipping Enable Human MTERF1 to Terminate Mitochondrial Transcription, Cell 141, 982-993 (2010).

Optimized for structure analysis of large molecular complexes at unprecedented rates.



From: P. Yuan, M.D. Leonetti, A.R. Pico, Y. Hsiung, and R. MacKinnon, Structure of the Human BK Channel Ca^{2+}-Activation Apparatus at 3.0 Å Resolution, Science 329, 182-186 (2010).

Optimized to support efficient exploration of vast numbers of specimens and conditions.



Source: Canted IVU21 undulator
Optics: - Double crystal mono
- Deflecting mirrors
- K-B focusing mirrors
E-range: 5 – 18 keV
Flux in focal spot: ~2×10^{13} ph/s
Focal spot min: 4 x 2 μm^2
Focal spot range: 5 – 100 µm

ADDITIONAL INFORMATION

This ALS-style crystal automounter at NSLS beamline X29 is fast in mounting crystals, but holds only 14 specimen in its dewar. By contrast, robotic systems based on six-axis robots, such as a CATS system from IRELEC, may hold hundreds of specimen, but are slow in mounting and retrieving them.

The remarkable flux from a IVU21 undulator will make it possible to complete data collections in a few seconds, thus leading to new crystallographic methods and practices.

To exploit this unique capacity we will resort to:

- A time-shared method of scheduling multiple projects for interleaved asynchronous data collections.
- A multi-stage robotic specimen change system including a fast crystal-mounting robot and one to replenish specimen pucks through the hutch wall.
- Software-assisted crystallographic decision making.
- Development by the crystallographic community of new sample preparation methods and specimen carrier formats.